Diatomic Air Species Spectra From The Infrared To The Vacuum Ultra Violet

David W. Schwenke[a]

[a]*NASA Ames Research Center, Moffett Field CA, 94035*

Abstract. As part of the HyperRad Project for the Fundamental Aeronautics Program at NASA, we have carried out first principle calculations of the spectra of N_2, N_2^+, O_2, O_2^+, NO, NO^+, CO, CN, and C_2. Many electronic states are considered so that we predict the spectrum from the infrared to the vacuum ultra violet. Rydberg states are explicitly included and high quality electronic wave functions are produced. Using these electronic wave functions, we compute the electric dipole, electric quadrapole and magnetic dipole transition moments as well as Spin-Orbit splittings and couplings. These are used in coupled ro-vib-electronic bound state calculations to produce bound-bound spectra. Above the lowest dissociation limit, the ro-vib-electronic levels become pre-dissociated, and we treat these levels using scattering theory to produce the bound-free and free-bound spectra. Novel diabatic states facilitate the nuclear dynamics calculations. All experimentally characterized bands are well reproduced, and a myriad of new states and bands are also predicted.

PACS: 31.15.ae, 31.15.ag, 31.15.aj, 31.15.vn, 31.15.xv, 31.50.Bc, 31.50.Df, 31.50.Gh, 33.13.Fm, 33.15.Kr, 33.15.Pw, 33.20.Bx, 33.20.Ea, 33.20.Kf, 33.20.Lg, 33.20.Ni, 33.20.Wr, 33.70.Ca, 33.80.Gj, 34.20.Cf.